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2. REPORT DATE

3. REPORT TYPE AND DATES COVERED

30 Sep 93 - 30 Jun 95

4. TITLE AND SUBTITLE

FINAL REPORT

5. FUNDING NUMBERS

AFOSR-TR-95

Work Station for Particle Simulations of

U. AUITIUNIS

Professor R. D. Murphy

61103D 3484/BS

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Department of Physics

Univ of Missouri-Kansas City

Kansas City, Missouri 64110

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING MONITORING AGENCY NAME (S) AND ADDRESSES AFOSR/NE

> 110 Duncan Avenue Suite B115 Bolling AFB DC 20332-0001

10. SPONSORING / MONITORING AGENCY REPORT NUMBER

F49620-93-1-0544

11. SUPPLEMENTARY NOTES

IVE. DISTRIBLITATION BYRELESS OF

19951002 016

APPROVED FOR PUBLIC RELEASE: DISTRIBUTION UNLIMITED

13. ABSTRACT (Maximum 200 words)

This is the final technical report for a DEPSCOR award for acquisition of computing equipment. Although there were some start-up difficulties, the final results are extremely good. The PI now has excellent research computing equipment which has been and will continue to be used for basic research underlying the technology goals of DOD. A research proposal will be submitted to AFOSR shortly.

DTIC QUALITY INSPECTED 5

14. SUBJECT TERMS			15. NUMBER OF PAGES
·			16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABS' RACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED

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August 30, 1995

Dr. Robert J. Barker Air Force Office of Scientific Research 110 Duncan Avenue Suite B115 Bolling AFB, DC 20332

Dear Dr. Barker:

Re: Grant No. F49620-93-1-0544

Enclosed please find the final technical report concerning the above grant. I would like to take this opportunity to thank you personally for your patient administration of this grant. I believe that the final results are fully consistent with the goals of the DEPSCOR program.

Please feel free to contact me at (816) 235-2509 if there is any additional information I can furnish.

Accesion For

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Sincerely yours,

R. D. Murphy Professor

enc

FINAL TECHNICAL REPORT

GRANT NUMBER F49620-93-1-0544

RESEARCH TITLE: WORK STATION FOR PARTICLE SIMULATIONS OF PLASMAS (DEPSCOR 92)

AUGUST 30, 1995

Principal Investigator:

Professor Richard D. Murphy

Department of Physics

University of Missouri - Kansas City

Kansas City, Missouri 64110 Telephone: (816) 235-2509

SUMMARY

This is the final technical report for a DEPSCOR award for acquisition of computing equipment. Although there were some start-up difficulties, the final results are extremely good. The PI now has excellent research computing equipment which has been and will continue to be used for basic research underlying the technology goals of DOD. A research proposal will be submitted to AFOSR shortly.

INTRODUCTION

This final technical report must begin with an expression of appreciation to the Air Force Office of Scientific Research for this award and for AFOSR's patient administration of this grant. Of particular importance was a crucial no-cost extension which permitted a very successful completion of the project in spite of considerable startup difficulties and delays.

These delays were due primarily to two causes. The first (and lesser) of these was that the manufacturer of most of the equipment, Digital Equipment Corporation (DEC), made in rapid succession a series of changes in their product lines; for example, in the few months between the submission of the proposal and the award of the grant, two major hardware items (workstation and printer) were discontinued. Although this (as well as long delays in shipping by and partial shipments from DEC) was a considerable inconvenience, the discontinuation of these products proved to be a good thing because they were replaced by higher-performance (and sometimes cheaper) hardware. The second and by far more serious delay resulted from the most difficult hardware "bug" the PI has ever encountered: it was ultimately traced to a defective component on the system board of the Alpha AXP machine. Because this bug was a) intermittent b) heat sensitive and c) on the CPU board, it produced puzzling symptoms and for a long time it was not even clear whether the problem was hardware, software, or both. The problem was finally diagnosed after considerable effort and corrected by DEC Field Service at no cost. All hardware and software are functioning flawlessly, and the machinery has run continuously for weeks at a time.

EQUIPMENT ACQUIRED

Page 6 of this report contains a list of the hardware and software acquired under this grant. The following is a brief description of the present equipment configuration. The primary installation consists of a DEC Alpha AXP 3000 Model 800 Hardware workstation powered by a Best Uninterruptible Power Supply and attached to a Digital LN08 DECLaser printer. This setup is located in the PI's computer lab, located in the basement of the Department of Physics. In the PI's office on the second story (and in the opposite corner) of the building is a smaller ancillary system consisting of a DEC Alphastation and a Hewlett-Packard LaserJet printer. Each system runs under OpenVMS and each has stand-alone computer capability. But the two machines are both connected via Ethernet and hence can communicate. They can also be configured as a DEC Cluster and share storage. Input/output can be accomplished through CD-ROM, DAT tape, or 3.5-inch floppy disk. Each machine has a single-user license from DEC, but the two independent setups make it possible for the PI and a graduate student to work simultaneously and independently. PC's (which were acquired from sources other than this grant) can be interfaced to each setup.

Software The DEC-supplied software (OpenVMS, DECNET, etc.) has been upgraded to the latest release level and will be so maintained for compatibility with campus computer facilities, which permit access to the Internet. The third-party graphics software (PV-Wave) is a powerful programming language which allows visualization, manipulation and analysis of multi-dimensional data.

RESEARCH ACCOMPLISHMENTS AND PLANS

Although the frustrating difficulties noted above have caused some delays in research output, there is progress to report. Furthermore, since the start-up problems have been resolved, the very powerful hardware will enable the PI to produce additional results shortly, as the following list shows.

- The PI's large-scale computer codes have been installed, converted to the Alpha hardware, and tested.
- 2) A moderately compute-intensive project has been completed and a paper ("Coulomb Energy and Madelung Constant of Calcite-type Lattices" by R. D. Murphy) has been submitted for publication.
- 3) A project in chemical kinetics (with a graduate student) is nearing completion.

 The graphics capability of PV-Wave and the DECLaser printer are being used to prepare publication-quality graphs. A joint manuscript should be submitted in September.
- 4) Calculations of the structure of liquid aluminum, a moderately computeintensive project which also requires PV-Wave, should yield a manuscript in October.
- 5) A proposal will be submitted to AFOSR (probably in October) involving highly compute-intensive neutral-gas aerodynamics and molecular dynamics plasma studies.

EQUIPMENT ACQUIRED

1)	DEC 3000 AXP Model 800 Workstation	\$35,496		
	(Machine, \$31,169 plus 3D graphics adapter, \$4,327)			
2)	DEC LN08 DECLaser printer	4,590		
3) Best Uninterruptible Power Supply		2,095		
4) PV-Wave Graphics Software		2,590		
5) DEC Alphastation Model 200		8,924		
6) DEC Monitor		840		
7) Hewlett-Packard LaserJet printer		1,417		
8) Setup costs		_1,222		
<u>Tot</u>	<u>tal</u>	\$57,174		
No	1) Items 1-5 were as approved in letter of June 2, 1995	from AFOSR.		
2) Items 6 and 7 are substitutions of like items for items approved in same				
	letter and are each (and in total) less than \$5000.			
	3) Item 8 (Setup costs) comprises several small items, n	ione over \$300,		
	principally Ethernet jacks and other connectivity h	nardware.		